Thermodynamics Properties of Real Polar Fluids From a Theoretical Equation of State

Y. Guevara and A. Laura Benavides
Instituto de Física
Universidad de Guanajuato
León, México

A. Estrada-Alexanders
Departamento de Física
Instituto de Fisica
Universidad Nacional Autónoma México
P.O. Box 20-364, México

We have calculated the thermodynamics properties of polar pure-substances in the fluid phase from a simple and analytical theoretical equation of state. Substances with a permanent dipole, quadrupole and/or octopole can be describe with great accuracy using as an effective intermolecular potential the following simple model: a superposition of a square-well and a point-multipole energy potential.

The equation of state is obtained from a statistical mechanics approach by means of perturbation theory in which, besides of the leading terms, an estimate of the rest of the series is included. Thus, we have been able to give an expression of the reduced Helmholtz free energy, which is explicit in the parameters that describe the effective intermolecular potential. These set of parameters (four for the case of polar substances) are adjusted from liquid-vapor equilibrium data and afterwards, the equation of state was used for the calculation of several thermodynamics properties such as pVT, heat capacities and speed of sound in both liquid- and gas-phase regions. The comparisons made for each substance studied are quite favorable.

In order to study the substances in a systematic way, we have classified them in families according to their permanent electric moment: dipolar, quadrupolar and octopolar fluids. Carbon monoxide, ethane, nitrogen, carbon dioxide, methane and tetrafluromethane were some of the substances studied.